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Monotonic Derivative Correction for Calculation of Supersonic Flows

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ABSTRACT

Aim of the study. This study examines numerical methods for solving the problems in gas dynamics, which are based on an exact or approximate solution to the problem of breakdown of an arbitrary discontinuity (the Riemann problem). **Results.** Comparative analysis of finite difference schemes for the Euler equations integration is conducted on the basis of an exact or approximate solution to the problem of an arbitrary discontinuity breakdown. An approach to the numerical solution of the Euler equations governing inviscid compressible gas flow is developed on the basis of the finite volume method and finite difference schemes for flow calculation of various degrees of accuracy. Calculation results show that monotonic derivative correction provides numerical solution uniformity in the breakdown neighborhood. On one hand, it prevents the formation of new extremum points, thereby providing monotonicity, but on the other hand, it causes smoothing of existing minimums and maximums and accuracy loss. **Conclusions.** The developed numerical calculation method makes it possible to perform high-accuracy calculations of flows with strong non-stationary shock and detonation waves and no non-physical solution oscillations on the shock wave front.

KEYWORDS
Computational fluid dynamics, finite volume method, Riemann problem, finite difference scheme, laval nozzle

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Introduction

In some cases, you must be able to calculate numerically supersonic flows with strong shock waves (Bulat & Chernyshov, 2016; Bulat & Volkov, 2016, Bulat & Upyrev, 2016). Application for solving such problems of traditional numerical methods often leads to unphysical solutions (Volkov, 2014; Bulat & Volkov, 2015; Bulat et al., 2015). This study examines the accuracy of the developed method for the numerical solution of the Euler equations governing

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inviscid compressible gas flow based on the finite volume method and finite difference schemes for flow calculation of various degrees of accuracy. The S.K. Godunov (1959) scheme (Einfeldt, 1988), Kolgan scheme (Kolgan, 1972), Roe scheme, Harten scheme, and Chakravarthy–Osher scheme (Osher, 1984; Osher & Chakravarthy, 1984; Sod, 1978) are used in the calculations; the order of accuracy of the schemes varies from 1st to 3rd (Capdeville, 2011). The comparison of various finite difference schemes in terms of accuracy and efficiency is demonstrated by the calculation of inviscid compressible gas flow in a Laval nozzle, with and without a starting shock wave (nozzle shock wave).

Model problems serve as a testing ground for verifying new methodological concepts and assessing the accuracy of the results obtained using software tools based on these concepts. An example is checking the developed concepts on the projection–evolution method, which is widely used in computational gas dynamics (Toro, 2009; Godunov, 1959; Kulikovskii, Pogorelov & Semenov, 2001; Roe, 1981). Calculation data provide the means for estimating the monotonicity and accuracy of the numerical method and for determining the presence of numerical diffusion and non-physical oscillations in the areas of steep gradients in the required functions (Donat & Marquina,1996). The problem of breakdown of an arbitrary discontinuity (the Riemann problem) has widespread application in the finite volume method when it comes to testing computational procedures and checking the accuracy of flow calculation schemes (Bulat & Bulat, 2015; Bulat et al., 2015).

To stop the iterative process, the obtained residual level is compared with the given degree of accuracy (convergence on machine accuracy is desirable but practically unattainable.) Accuracy estimation methods are based either on graphical representation of the history of iterative process convergence or on theoretical examination of residual behavior. These methods depend on the type of convergence (monotonic, oscillating, combined). For this purpose, a hierarchy of grids with various decreasing space and time steps is used.

Grid dependence of the solution can be checked by solving the problem on a sequence of grids, where the step decreases by a certain value (by half, for example) moving down the grid hierarchy.

This study solves numerous problems associated with the simulation of supersonic flow of an inviscid compressible gas through a Laval nozzle, with and without a starting shock wave. The obtained model numerical solutions are then compared with the published model solutions, which makes it possible to assess the accuracy of the finite difference schemes. Monotonic derivative correction provides numerical solution uniformity in the breakdown neighborhood. On one hand, it prevents the formation of new extremum points, thereby providing monotonicity, but on the other hand, it causes smoothing of existing minimums and maximums and accuracy loss.

The Riemann problem

The problem of breakdown of an arbitrary discontinuity consists in solving the Euler equations in the interval $-\infty < x < +\infty$ under specific initial conditions characterized by a constant state in the half-plane $-\infty < x < 0$ (index L) and in the half-plane $0 < x < +\infty$ (index R). The initial conditions for the Euler equations are as follows (physical variables are used):

where is a vector of gas-dynamic variables (density, velocity components, total energy per unit of volume).

A membrane positioned at the point x = 0 separates two gases at different pressures, with different densities and velocities. Air with specific heat ratio $\gamma = 1.4$ is chosen as the operating medium.

At the time t = 0, a discontinuity of gas-dynamic parameters is formed at the point x = 0, which corresponds to the position of the splitter plate. At the time t = 0, the splitter plate is instantly removed. The arbitrary discontinuity breaks into several discontinuities, each of which is a shock wave or an expansion wave, depending on the initial conditions. Possible solutions contain an expansion fan, contact discontinuity, and a shock wave, which split the area into four subareas with constant parameter values. The exact solution to the problem of breakdown of an arbitrary discontinuity comes down to solving a system of nonlinear algebraic equations derived from the conservation law. This solution is examined in many research papers (Toro, 2009; Kozhemyakin, Omel'chenko & Uskov, 1999).

Existing solution methods

In the S.K. Godunov (1959) method gas parameters are approximated by piecewise constant distributions on the selected grid such that within each cell, these parameters remain constant and equal to the average values over the cell. Piecewise constant field evolution over a fairly short time interval, which is determined using the exact solution of the Riemann problem in each cell, is used to find average cell values on a new layer in time. By repeating this procedure step by step, the dynamics of flow variation in time are calculated.

Piecewise constant and piecewise polynomial distributions of functions in a discrete cell, with certain restrictions on the coefficient values of the corresponding polynomials, are used to develop highly accurate S.K. Godunov (1959) -type numerical methods. One of the difficulties encountered is uncertainty in selecting slope values for these distributions. In these cases, the breakdown of an arbitrary discontinuity causes it to lose its self-similarity. Finding the exact solution to the Riemann problem with random initial conditions becomes complicated (for the generalized Riemann problem, in which flow parameters on the left and right side of the discontinuity are variables). The solution of a non-self-similar problem can be avoided by instead solving a problem that is an approximation of the self-similar one.

The use of piecewise linear approximations requires derivatives to be determined in each computational cell. In smooth flows, another approach can be applied, where derivatives of each layer in time are approximated by the calculated average values. Applying this approach to flows with discontinuities results in major errors. In practice, derivatives are not approximated but are calculated using data on the nature of the flow.

The S.K. Godunov (1959) method can be relatively easily generalized to a multivariate case. Flow parameters in each grid cell are considered constant (the flow in a cell is assumed to be homogeneous). Flow development comes down to the interaction of homogeneous flows at cell edges (ignoring flow interaction at cell apexes). This approach involves calculating the interaction of two homogeneous gas flows, which are initially separated by a certain plane. The

solution of a 3D problem comes down to the solution of a one-dimensional problem along the normal to the separating plane.

A previous study (Kulikovskii, Pogorelov & Semenov, 2001) introduces an exact solution to this problem. Finding such a solution is crucial because it makes it possible to consider the properties of a fairly standard medium when an approximation by two-term equations of state is applied. One-parameter approximations of the equation of state do not ensure the transmission of properties of various media on the left and right side of the discontinuity. For some types of equations of state, the solution of the Riemann problem is not the only one. The solution has a complex, non-classical structure or disturbs the hyperbolicity of a system of equations

The approaches described in (Roe, 1981; Einfeldt, 1988; Donat & Marquina, 1996) are among the most widespread methods that are based on approximated solutions to the problem of breakdown of an arbitrary discontinuity. In some studies (Osher, 1984; Osher & Chakravarthy, 1984), when an arbitrary discontinuity breaks down, a shock wave is replaced by a compression wave, which results in a system of equations with monotonic solutions. In another study (Einfeldt, 1988), breakdown is treated using two Jacobians, one for the left node and one for the right node, to construct a single Jacobian from the simple waves of the left Jacobian moving to the right and those of the right Jacobian moving to the left. A previous study examines only expansion and compression waves. The Roe scheme (Roe, 1981) is based on assigning explicit formulas to determine linearized values that make up a Jacobian (primitive variables are used). However, the Roe scheme has a drawback: it allows the presence of an expansion shock wave at the sonic point. This can be avoided by adding extra viscosity, thereby modifying eigenvalues in the neighborhood of sonic points.

The Roe method (Roe, 1981) is based on an exact solution to the Riemann problem for a specially linearized system of equations. The solution consists of moving discontinuities separated from each other by areas with constant variable values. Such a solution is unusual because it preserves the non-linear Rankine–Hugoniot relations on a single shock wave and the relations on a single tangential discontinuity. The Roe method provides a means for building finite difference schemes for conservative hyperbolic sets of equations.

In the S. Osher (1984) method, an approximate solution to the Riemann problem is built for a quasilinear system of equations and is basically a combination of Riemann waves only.

Numerical methods

Mathematically, the problem of breakdown of an arbitrary discontinuity is a Cauchy problem with initial conditions for conservation laws that determine the movement of a compressible gas, with the initial distribution of gas parameters in the form of piecewise constant functions.

In the S.K. Godunov (1959) method, piecewise constant distributions of functions are used to describe an instantaneous state of a moving medium (flow parameters are considered constant within each control volume). Further development of flow approximation, which consists of many elementary homogeneous flows in time, is determined by the solution of the Riemann problem at the edges of control volumes. It is possible to describe the whole variety of discontinuity configurations using a relatively simple scheme.

Discontinuity velocities and flow parameters in smooth areas between discontinuities can be determined by simple mathematics.

The S.K. Godunov (1959) finite difference scheme is a conservative scheme of first-order accuracy. It is widely applied in various problems involving numerical simulation of compressible gas dynamics. The S.K. Godunov (1959) scheme uses approximate viscosity, which means that artificial viscosity is not required for strong discontinuity calculations. During the calculation of weak discontinuities such as expansion waves, approximation error becomes significant, which manifests itself as strong smearing (the less the Courant number, the stronger is the smearing). The restriction on time step follows from the condition that waves formed after the discontinuity breakdown at the edge of the control volume should not reach its center or, with a less strict restriction, its other edge. In the area where strong shock waves interact, the S.K. Godunov (1959) method displays numerical damping properties similar to those of the application of artificial quadratic viscosity (Kulikovskii, Pogorelov & Semenov, 2001). The S.K. Godunov (1959) methods based on the solution of the Riemann problem by the Roe method have numerical linear viscosity. During the simulation of strong shock waves, the Courant number needs to be decreased from 1 to 0.2 to ensure stability of calculations.

The data required for flow calculation in the Godunov method come down to using the state that formed after the discontinuity breakdown at the edge of the control volume. Solving the Riemann problem is demanding; yet, the Godunov method only uses a part of the obtained data.

Godunov's numerical methods constructed using the exact solution of the Riemann problem provide the means for calculating shock waves of arbitrary intensity with the Courant number close to 1 ($0.8 < C < 1$).

Numerical methods based on approximate solutions to the Riemann problem rely on separate exact elementary solutions to the Riemann problem (moving discontinuities in the Roe method or Riemann waves in the S. Osher (1984) method). Various conclusions and additions are discussed in previous studies.

Nozzle flow

Let us consider the flow of inviscid compressible gas in a channel with a variable cross-section area (a Laval nozzle). The nozzle section is described by the dependence y = [(1 + x2)/π]1/2, where x is in the interval [–0.3.1]. Air (γ = 1.4) is taken as the operating medium. Details on the computational procedure have been provided in previous studies (Volkov, 2005; Volkov, 2006). Indices 00 correspond to the parameters of the flow in the receiver, while the index ∞ corresponds to the parameters of the flow in the surrounding medium

The nozzle flow mode is determined by the correlation between the pressure at the nozzle exit, p2, and the pressure in the tank, p1. In alternative 1 (pressure drop below critical, p2/p1 > 0.528), a flow mode with back pressure is implemented, where pressure buildup of the over-expanded flow to the external pressure is performed through the nozzle shock wave. In alternative 2 (pressure drop is above critical, p2/p1 < 0.528), gas is sustainably accelerated from subsonic velocity at the point of entry to a certain velocity at the throat, which is dependent on the given pressure drop. The gas is then stagnated.

At the nozzle entry, the total pressure and total temperature are set. The settings for boundary conditions at the nozzle exit depend on the gas flow mode. With subsonic flow at the exit, the static pressure is set equal to the external pressure. Other parameters are determined through extrapolating variables from the internal cells of the computational domain. Supersonic flow requires no additional boundary conditions at the exit.

Calculations are performed on a 100-cell grid. The Courant number is assigned the value CFL (Courant−Friedrichs−Lewy) = 0.95. A stationary solution to the problem can be achieved using the relaxation method.

In alternative 1 (p2/p1 > 0.528), stagnation pressure (p1 = 106 Pa) and stagnation temperature (T1 = 300 K) are set at the nozzle entry and static pressure (p2 = 8•105 Pa) is set at the nozzle exit. At the entrance to the computational domain, the flow is subsonic. At the convergent section of the nozzle, the flow is accelerated, reaching sonic velocity at the throat, and it keeps moving at supersonic velocity. At the divergent section of the nozzle, a straight shock wave is formed, beyond which the flow becomes subsonic.

In alternative 2, gas is accelerated at the subsonic section and stagnated in the supersonic section.

Calculations are required to compare various flow calculation schemes (Yeom & Chang, 2013; Su, 2014). Results of the numerical simulation processed in the form of pressure–coordinate x-dependence are shown in the Fig. 1 (Courant number 0.98) and Fig. 2 (Courant number 0.25). Finite difference schemes smear out the discontinuity across 1–2 computational cells, preserving the monotonic nature of the solution.

In the presence of a nozzle shock wave (Fig. 1), the Chakravarthy–Osher scheme produces results closest to the exact solution. The Godunov scheme requires 0.03479 s of estimated time (12 time steps) to reach a stationary state, the Kolgan scheme requires 0.03401 s (12 steps), the Roe scheme requires 0.01999 s (6 steps), the Harten scheme requires 0.01975 s (5 steps), and the Chakravarthy–Osher scheme requires 0.01968 s (5 steps).

In a supersonic flow mode (Fig. 2), all finite difference schemes produce similar results. The Godunov scheme requires 0.007257 s of estimated time (14 time steps) to reach a stationary state, the Kolgan scheme requires 0.008151 s (15 steps), the Roe scheme requires 0.009545 s (18 steps), the Harten scheme requires 0.006941 s (12 steps), and the Chakravarthy–Osher scheme requires 0.006938 s (10 steps).

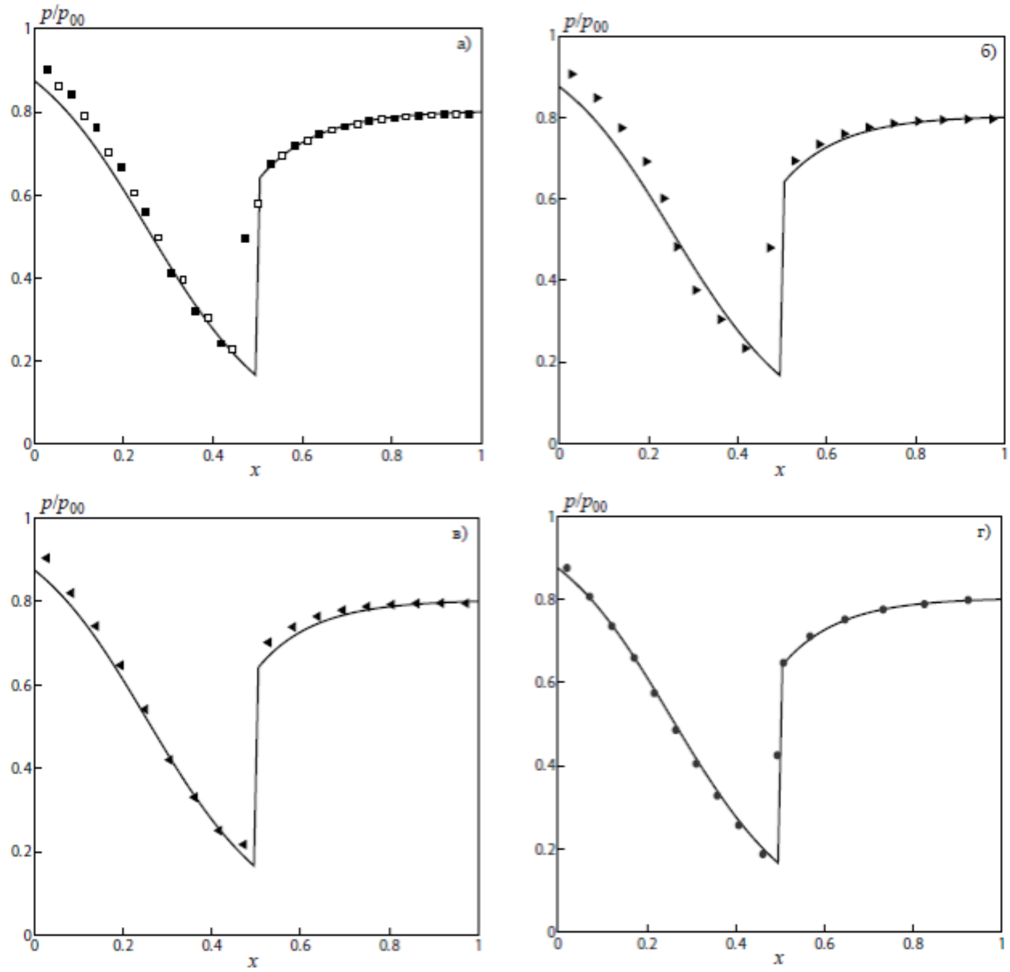

Figure 1. Pressure distribution along the *x* coordinate with p_{00} = 10^6 Pa, T_{00} = 300 K, p_∞ = $8{\cdot}10^5$ Pa.

Icons ■ and □ correspond to the results obtained using the Godunov scheme and the Kolgan scheme, respectively (a); ► – using the Roe scheme (b); ◄ – using the Harten scheme (c); ● – using the Chakravarthy–Osher scheme (d)

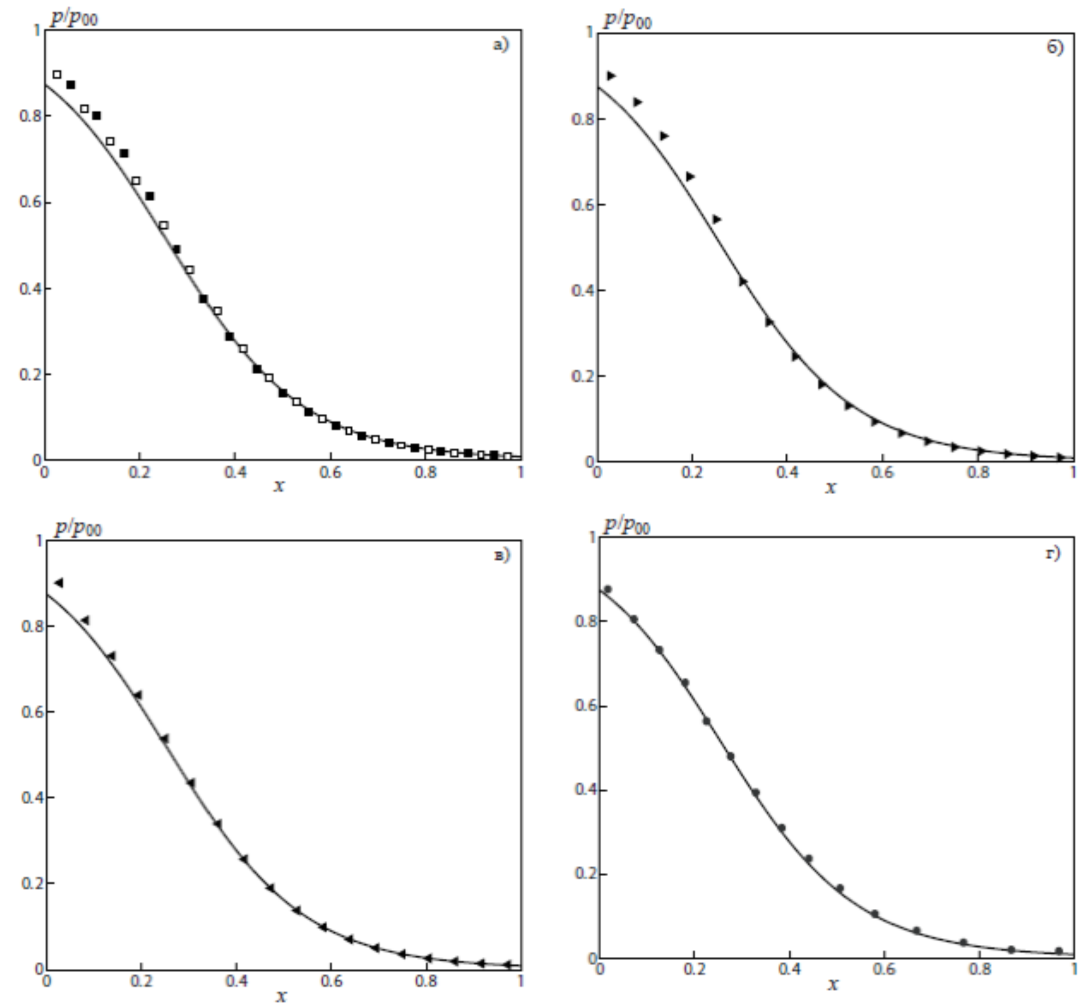

Figure 2. Pressure distribution along the *x* coordinate with $p_{00}=10^8$ Pa, $T_{00}=300$ K, $p_\infty=8\cdot10^5$ Pa.

Conclusions

It is possible to assess the accuracy and convergence rate of a scheme by comparing solutions of model problems with exact solutions. Construction of exact model solutions is a crucial element in the general routine of numerical algorithm construction.

Comparative analysis of finite difference schemes for the Euler equations integration is conducted on the basis of the exact or approximate solution to the problem of an arbitrary discontinuity breakdown. The accuracy and effectiveness of various finite difference schemes are demonstrated by calculating the inviscid compressible gas flow in a Laval nozzle. The Godunov scheme, Kolgan scheme, Roe scheme, Harten scheme, and Chakravarthy–Osher scheme are used in the calculations; the order of the schemes varies from 1st to

3rd. Calculation results show that monotonic derivative correction provides numerical solution uniformity in the breakdown neighborhood. On one hand, it prevents the formation of new extremum points, providing monotonicity, but on the other hand, it causes smoothing of existing minimums and maximums and accuracy loss.

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Disclosure statement

No potential conflict of interest was reported by the authors.

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